High Production Volume (HPV) Challenge Program

Data Summary and Test Plan
for
2-amino-2,3-dimethylbutanenitrile
CAS# 13893-53-3

Prepared by

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A. INTRODUCTION

On November 22, 1999, Cytec Industries Inc. (Cytec) voluntarily agreed to participate in the Environmental Protection Agency's (EPA) High Production Volume Chemical Challenge Program. By participating in this program, Cytec agreed to assess the adequacy of existing data, design and submit test plans to fill data gaps where necessary and appropriate, provide test results, and prepare summaries of the data characterizing each chemical.

The sponsored chemical addressed in this test plan is 2-amino-2,3-dimethylbutanenitrile, (CAS # 13893-53-3).

B. GENERAL SUBSTANCE INFORMATION

Chemical Name: 2-amino-2,3-dimethylbutanenitrile

Chemical Abstract Service Registry Number: CAS # 13893-53-3

Common Name: aminonitrile

Chemical Formula: $C_6H_{12}N_2$
Structural Formula: CH_3- C (CH_3)(NH_2) CH(CH_3) -CN
Molecular Weight: 112.2

C. EXPOSURE INFORMATION

Pursuant to USEPA's Guidance for Testing Closed System Intermediates for the HPV Challenge Program, 2-amino-2,3-dimethylbutanenitrile meets the definition of an isolated intermediate with controlled transport, i.e. transported to a limited number of locations which use the chemical in a controlled way as an intermediate with a well-known technology. Thus, the following information is being provided to support the information requirements necessary to meet exemption claims for reduced SIDS testing based on exposure considerations.

Cytec manufactures in excess of 1 million pounds/year of 2-amino-2,3-dimethylbutanenitrile under an extensive USEPA 5(e) Consent Order/SNUR. As such, there are prescribed conditions for its manufacture, processing, distribution, use and disposal. As a result, there is low potential for exposure of humans or the environment. In the work place, potential worker exposure is carefully controlled.

Manufacture: Cytec manufactures 2-amino-2,3-dimethylbutanenitrile at only one location as identified in the USEPA 5(e) Consent Order/SNUR. The manufacturing employs a "closed process" system and mandated requirements for personal protective equipment. The batch process consists of mixing the reactants and then extracting the 2-amino-2,3-dimethylbutanenitrile with toluene. Then the mixture is purified by boiling under vacuum to remove any light impurities. All process vessels than contain 2-amino-2,3-dimethylbutanenitrile

are vented to a plant flare via a seal pot. The low vapor pressure of 2-amino-2,3-dimethylbutanenitrile at process conditions combined with the combustion in the flare results in virtually no emissions of 2-amino-2,3-dimethylbutanenitrile to atmosphere. The only waste stream from the process is an aqueous purge stream that is disposed using Class I deepwell injection.

The three reactants which form 2-amino-2,3-dimethylbutanenitrile are mixed in an aqueous solution in a 7500-gal reactor. The vent from which is routed to a seal pot which vents to a flare. Once the reaction is completed, the 2-amino-2,3-dimethylbutanenitrile is extracted from the aqueous solution utilizing toluene. The organic phase resulting from this extraction, which contains the majority of the 2-amino-2,3-dimethylbutanenitrile, is pumped, with a sealless magnetic drive type pump, to a 4,400 gal drying vessel. This mixture is then vacuum distilled to remove the water and excess toluene, which is condensed for recycling. The non-condensables are routed to the flare via the seal pot. The contents of the dryer is then pumped, with a sealless magnetic drive type pump, to product storage. The vent from the storage tank is also routed via the seal pot to the flare. The aqueous phase from the reactor is pumped to a 4,800 gal extractor vessel, where it is again extracted with toluene to recover additional 2-amino-2,3-dimethylbutanenitrile. The majority of the remaining aqueous phase is then pumped, with a sealless magnetic drive type pump, to the reactor to serve as the starting aqueous solution for the next batch. A portion of the aqueous solution is pumped to the seal pot from where it is disposed using Class I deepwell injection. The product 2-amino-2,3-dimethylbutanenitrile is loaded into dedicated containers which are vapor equalized with the product storage tank. The loading and vapor return hoses are blown with nitrogen into the container and storage tank before disconnecting to minimize potential exposure. The control valves in 2-amino-2,3-dimethylbutanenitrile service are rotary type with a packing seal. All the pumps in the in the 2-amino-2,3-dimethylbutanenitrile plant are sealless magnetic drive type pumps except for the seal pot liquid pumps which have double mechanical seals with a pressurized barrier fluid.

The entire 2-amino-2,3-dimethylbutanenitrile plant is within secondary containment which drains to a containment sump. This material is disposed using Class I deepwell injection. Process equipment is decontaminated for routine maintenance by flushing to the seal pot from where it is disposed using Class I deepwell injection.

Extensive automation of the process using remote process control computers and terminals permits monitoring and control of the process from a process control room. Thus the time the operator is in the process area is limited, thereby minimizing potential exposure time. Additional worker activities during the process may include collection, analysis, and disposal of samples, routine maintenance, clean-up of equipment, and tank truck loading. The production equipment is maintained utilizing a mechanical reliability program to prevent failures.

2-amino-2,3-dimethylbutanenitrile is a liquid of low vapor pressure at ambient temperatures, so the risk of vapor inhalation is relatively small. However, some concentration of HCN (hydrogen cyanide) will exist above the liquid. HCN is a quick acting poison in that it is rapidly absorbed through unbroken skin and especially through the eyes. Thus, the facility is continuously monitored for HCN (a hazardous decomposition product of 2-amino-2,3-dimethylbutanenitrile) at a level not to exceed 5 ppm. There is one operator per shift who covers the 2-amino-2,3-

dimethylbutanenitrile plant, ~30% of their time is in the 2-amino-2,3-dimethylbutanenitrile area. There is also a loader on some days who spends ~2 hrs unloading raw materials and loading 2-amino-2,3-dimethylbutanenitrile. Supervisory and maintenance people (5-6 people) spend ~ 4 hrs/week in the area.

Processing: The material is made on site as 80% 2-amino-2,3-dimethylbutanenitrile in 20% toluene and is stored onsite until delivered to the sole customer. It is not further processed on-site or used for any other application.

Distribution (Transport): The material is transported by Cytec's customer under strict safe transportation guidelines, by truck, in DOT 51 specification containers designed, constructed and tested in accordance with ASME Code, Section VIII, Div 1 for lethal service and UCC COP-1-22. The tank container framework structure is in accordance with ISO 1496/111 and provides physical protection from tanker appurtenances. The tank container is labeled with the following placards: FLAMMABLE and POISON UN2929. In addition, the tanker is marked: INHALATION HAZARD, Toxic liquid, Flammable Organic, 2-amino-2,3-dimethylbutyronitrile in toluene. The tanker chassis is supplied by Quality Carriers. The annual volume transported to the single use site is 1 to 4 million pounds.

These specially designed trucks are equipped with personal protective/emergency response equipment, GPS locators, emergency communication equipment, are manned by two specifically trained and qualified shift drivers, and only drive during specified dawn to dusk daylight hours under favorable weather conditions and along prescribed routes. Prior to departure of each loaded tanker, the shift superintendent at the plant conducts an out-bound inspection of the drivers personal emergency equipment and gear, ensures that all of the emergency equipment tool boxes are in place and verifies that the dome cover has an appropriate seal and that there are no visible deficiencies or leaks coming from with the tractor or the chassis/tanker. Emergency response personnel in each area that the material is transported are aware of the hazards of the material, the transport routes, and necessary emergency response guidelines. The receiving plant conducts an in-bound safety inspection for each shipment arriving at the plant.

Customer use: It is manufactured for one customer (BASF Corporation) is used solely as a raw material for the production of a class of herbicides of very low toxicity and is not sold as an article of general commerce or transferred to any contract manufacturer.

The receiving plant conducts an in-bound and out-bound safety inspection for each shipment. Inspections include tanker check for integrity using hand held cyanide detectors and general tractor and trailer condition. Brake systems, lights, trailer seal, toolbox seals, labelling and placards are all checked. Drivers are checked for attendance safety school.

2-amino-2,3-dimethylbutanenitrile is unloaded at the customer site into a stainless steel storage tank that is vented to a caustic scrubber for removal of any trace quantities of HCN, the vent gas is further processed in one of two RCRA incinerators.

2-amino-2,3-dimethylbutanenitrile is charged to one of two herbicide batch manufacturing processes. It is consumed by the processes or dissociated to its component parts (MIPK, HCN

and ammonia) which are then subsequently removed from the process streams by caustic scrubbers and distillation. Both processes are closed systems with process fumes being scrubbed for cyanide removal and subsequently further processed by incineration.

All process aqueous waste streams and organic waste streams are destroyed in RCRA incinerators through closed handling systems. The herbicide processes, as well as the incineration areas, are continuously monitored for HCN (a hazardous decomposition product of 2-amino-2,3-dimethylbutanenitrile) at a level not to exceed 4 ppm by stationary analyzers that monitoring multiple points throughout the units. A separate HCN monitor is installed exit the scrubbers to alarm at 4ppm HCN.

There are nine operators and one supervisor per shift who cover the two herbicide manufacturing processes. Extensive automation of the process using remote process control computers and terminals permits monitoring and control of the process from a process control room. Thus the time the operator is in the process area is limited, thereby minimizing potential exposure time. While in the process and unloading areas, operating personnel wear the proper personal protective equipment including personal HCN continuous monitors. Additional worker activities during the process may include collection, analysis, and disposal of samples, routine maintenance, clean-up of equipment, and tank truck unloading. The production equipment is maintained utilizing a mechanical reliability program to prevent failures.

In addition, the herbicide made is for commercial industrial use only and is not made available to the general consumer retail market.

Disposal: Aqueous wastes containing 2-amino-2,3-dimethylbutanenitrile are co-mingled with a wastestream that is maintained at a pH of at least 10 by the addition of caustic to chemically decompose the material to a wastestream concentration of <10 ppm, followed by injection of the resultant constituents into Class I deepwell injection waste disposal wells, licensed by the state in which the plant resides and under authority delegated by the EPA. A "no migration" petition, approved by EPA, evidences the agency's conclusion that this disposal method will not result in any environmental release for a period of at least 10,000 years. Effluent monitoring has never shown any detectable quantities of 2-amino-2,3-dimethylbutanenitrile monitored over a ten year period.

D. SUMMARY TABLE OF AVAILABLE DATA

CAS# 13893-53-3	Study Date	Results	Data Acceptable
Physical/Chemical Characteristics			
Melting Point	2001	Not Applicable	Yes
Boiling Point	2001	186.88 °C (with decomposition)	Yes
Vapor Pressure	2001	0.6 mm Hg @ 25 °C	Yes
Partition Coefficient	2001	Log Kow = 0.87	Yes
Water Solubility	2001	$1.07 \times 10^{+5}$ mg/L @ 25 °C	Yes
Environmental Fate			
Photodegradation	2001	For reaction with hydroxyl radical, predicted rate constant = 2.888×10^{-12} cm^3/molecule-sec Predicted half-life = 44.443 hours	Yes
Stability in Water	2001	Partially hydrolyzes in water producing HCN. Aqueous wastes containing 2-amino-2,3-dimethylbutanenitrile chemically decompose when commingled with a wastestream that is maintained at pH 10.	Yes
Fugacity	2001	Predicted distribution using Level III Fugacity Model: Air: 0.158% Water: 46.2% Soil: 53.5% Sediment: 0.0913%	Yes
Biodegradation	2001	Not estimated to be biodegradable	Yes
Ecotoxicity			
Acute Toxicity to Fish	1984	Lepomis macrochirus: LC50 (96 hr) = 0.75 mg/L NOEC (96 hr) = 0.56 mg/L	Yes
Acute Toxicity to Invertebrates	1984	Daphnia magna LC50 (48hr) = 6.9 mg/L NOEC (48 hr) = 3.2 mg/L	Yes
Acute Toxicity to Algae	1984	Selenastrum capricornutum: EC50 (96 hr) = 0.36 mg/L NOEC (96 hr) = 0.10 mg/L	Yes
Mammalian Toxicity			
Acute Toxicity	1989 1989 1988	Rat: oral LD50 = 83 mg/kg Rabbit: dermal LD50 = 23 mg/kg Rat: inhalation LC50 = 67 – 79 ppm (4 hr); 87 –97 ppm (1 hr)	Yes
Repeat Dose Toxicity	1984	(28 day) rat: NOEL = 3 mg/kg	Yes
Developmental Toxicity		Surrogate Data	Yes
Reproductive Toxicity		No data	**No Data**
Genetic Toxicity: Gene Mutations	1983	Salmonella typhimurium: Not mutagenic	Yes

Genetic Toxicity: Chromosomal Aberration		No data	**No Data**

E. TEST PLAN FOR 2-amino-2,3-dimethylbutanenitrile (CAS# 138893-53-3)

For closed system intermediates, such as 2-amino-2,3-dimethylbutanenitrile, a reduced test plan package reflecting the information needed to evaluate the hazards in case of an accident is considered the appropriate level of testing for screening purposes. This is because exposures resulting from chemical accidents are likely to be of relatively short versus chronic duration. In addition, chronic exposures to 2-amino-2,3-dimethylbutanenitrile following an accident are not likely due to its rapid degradation to CN^-, ammonia, and methyl isopropyl ketone; and chronic exposures are not likely in the workplace due to the stringent safety measures employed during manufacture.

This safely handled material is manufactured and transported under strict safeguards to eliminate any potential for human or environmental exposure. Conditions in which humans or the environment could be potentially exposed to 2-amino-2,3-dimethylbutanenitrile are limited and not likely to occur. As such, the reduced testing appropriate for 2-amino-2,3-dimethylbutanenitrile consists of the data already obtained, the Screening Information Data Set (SIDS) minus the tests for reproductive toxicity, developmental toxicity and chromosomal aberration. Filling these endpoints will not contribute to a greater understanding of the acute hazards to human health or the environment associated with this material and will not be of value to the safe manufacture and handling of this material.

Thus, due to the low potential for human (closed system manufacture, personal protective equipment, limited number of workers, and no public exposures) or environmental (deep well injection of wastes) exposure and the high degree of acute toxicity associated with this material, additional tests to elucidate the toxic potential of 2-amino-2,3-dimethylbutanenitrile for those endpoints not already assessed are not warranted.

CAS# 13893-53-3	**Data Available**	**Data Acceptable**	**Testing Required**
Study	Y/N	Y/N	Y/N
Physical/Chemical Characteristics			
Melting Point	Y	Y	N
Boiling Point	Y	Y	N
Vapor Pressure	Y	Y	N
Partition Coefficient	Y	Y	N
Water Solubility	Y	Y	N
Environmental Fate			
Photodegradation	Y	Y	N
Hydrolysis	-	-	N